

## An Evaluation of Temperature Variation Resistivity of Alkali Metal Doped Fluoride $K_3C_{60}$

DEEPAK KUMAR\*, V. K. VERMA\*\* and L. K. MISHRA

Department of Physics,  
Magadh University, Bodh-Gaya, Bihar, INDIA.

\*\*Department of Physics,  
Gaya College Gaya, Bihar, INDIA.

\*C/o Sri Rambilas Singh,  
Loko Colony, Q. No 308/A , Gaya, Bihar, INDIA.

(Received on: February 22, 2013)

### ABSTRACT

Using the theoretical formulism developed by L. *Pintschovius*. (1996), we have presented a method of evaluation of temperature dependent resistivity  $\rho_{e-ph}$  (electron-Phonon),  $\rho_{er}$  (Inter molecular Phonon),  $\rho_{ra}$  (Intra molecular Phonon) , total resistivity  $\rho(T)$  and  $\rho_{diff}$  (Difference between theoretical-experimental) for  $K_3C_{60}$  fluoride. Our theoretical results are in good agreement with experimental data and also with other theoretical workers.

**Keywords:** Normal state resistivity, Electron-phonon, Inter-molecular Phonon, Intra-molecular Phonon, Alkali metal doped fluoride, electron doped cuprates, dimensionally crossover.

### 1. INTRODUCTION

In this paper we have presented the method of evaluation of temperature dependent resistivity due to electron-phonon interaction ( $\rho_{e-ph}$ ), temperature variation of total resistivity  $\rho(T)$  and temperature variation of  $\rho_{diff}$  (measured  $\rho$ -calculated  $\rho$ ) for  $K_3C_{60}$  fluoride. As we all know that electrical resistivity  $\rho$  can be caused by various scattering mechanism. An important

mechanism is the electron- phonon interactions. In this mechanism electrons are scattered under the simultaneous excitations of phonons. The equally important mechanism is electron-electron interaction. The contribution of these two mechanisms<sup>1,2</sup> goes to zero as  $T \rightarrow 0$ .

In case of metal, electron- phonon scattering is the major source of temperature dependent resistivity. The other scattering mechanisms are electron impurities

scattering due to defects, grain and disorder regions. Unfortunately, all these mechanisms give temperature independent contributions. For the evaluation of resistivity of alkali metal doped fluoride one uses zero temperature scattering rate related to upper critical magnetic field  $H_{c2}(0)$ <sup>3</sup>, modified BCS theory and the use of Matsubara gap function<sup>4</sup>, which uses to square well potential model. In these calculations the zero temperature resistivity is expressed as

$$\rho_{(0)} \tau^{*-1} \omega_p^{-2} \quad (1)$$

Here  $\omega$  is the plasma frequency, is the impurity scattering time defined as  $(1+\lambda)$  is the scattering factor, appears in the modified BCS theory and  $\tau$  the scattering time. In this calculation the zero temperature resistivity has been calculated by keeping the parameter<sup>5</sup>

$$\begin{aligned} T_C &= 22\text{K}, \\ V_F &= 1.9 \times 10^7 \text{ cm/sec}, \\ \omega_p &= 1.2 \text{ eV}, \\ H_{C2}(0) &= 49 \text{ Tesla}, \\ \tau &= 1.23 \times 10^{-14} \text{ sec}^{-1} \end{aligned}$$

These all parameters are taken from the reference<sup>6,7</sup>.

Our theoretical evaluated results of temperature variation resistivity  $\rho_{e-ph}$  (due to electron-phonon),  $\rho_{er}$  (due to intermolecular phonon) and  $\rho_{ra}$  (due to intra molecular phonon), we have taken the intermolecular frequency  $\omega_{er} = 9\text{K}$  and intramolecular frequency  $\omega_{ra} = 1455\text{K}$ . Our theoretical results shows that  $\rho_{er}$  increases linearly with  $T$  and  $\rho_{ra}$  increases exponentially with  $T^*$ . When these resistivity are combined together to calculated resultant resistivity  $\rho_{e-ph}$  then it was found that  $\rho_{e-ph}$  varies exponentially

with low  $T$  and linearly with high  $T$ . Our other calculation  $\rho_{diff}$  shows that it has a power dependence of temperature as low  $T$  and it becomes almost saturated at high  $T$ .

## 2. MATHEMATICAL FORMULA USED IN THE EVALUATION

Now one can estimate zero temperature limited resistivity with the help of zero temperature elastic scattering rate and plasma frequency. The zero temperature scattering rate is related through the upper critical magnetic field  $H_{C2}(0)$ . Following the two square well analysis of Elishberg theory, Carbotte<sup>8</sup> suggested that the strong coupling correlation are important and a rescaling factor  $(1 + \lambda)$  appears in the modified BCS results. The Mastubara gap function which is related with upper and the factor critical magnetic field yields<sup>9</sup>

$$\left(\frac{1+\lambda}{\lambda-\mu^*}\right) = 2\pi \left(\frac{T}{T_C}\right) \sum_{m=0}^{N_C} \frac{1}{\chi_m^{-1} (\bar{\omega}_m) - (2\tau)^{-1}} \quad (2)$$

$\bar{\omega}_m$  Being the Mastubara frequency, within the standard two-square-well model is  $\bar{\omega}_m = \omega_m (1 + \lambda) + (2\tau)^{-1} (\text{sgn } \omega_m)$ ,  $\lambda$  the electron-phonon coupling strength with cut off at  $N_C$  and the scattering time. In this approximation,  $N_C$  follows

$$N_C = (1/2) [(\omega/\pi T) + 1] \quad (3)$$

$\mu^*$  being the normalized Coulomb repulsive parameter and the factor  $\chi_m$  appearing in (1) with

$$\phi = \frac{q\sqrt{\xi^*}}{[(2m+1)\pi] \frac{T}{T_C} + \left[\frac{1}{2\tau^*}\right]} \quad (4)$$

The upper critical magnetic field is related through

$$\xi^* = \frac{1}{2} e H_{c2}^* v_F^{*2} \quad (5)$$

The physical quantities appearing in (1) – (5) involve renormalized value as

$$H_{c2}^* = \frac{H_{c2}}{(1+\lambda)T_c} \quad (6)$$

$$v_F^* = \frac{v_F}{(1+\lambda)T_c} \quad (7)$$

and impurity scattering time

$$\tau^* = \frac{\tau}{(1+\lambda)T_c} \quad (8)$$

The above derived equation differ from the BCS limit, as the renormalizations in  $\xi^*$ ,  $v_F^*$ ,  $H_{c2}^*$  and  $\tau^*$  are introduced. These expressions are valid for any impurity concentration described in (1) - (5) by scattering time. In the present analysis, Pauli limit has been neglected as an approximation<sup>9</sup>, due to relatively small value of  $dH_{c2}/dT \left[ 1/[(1+\lambda)] \right]$  in alkali metal intercalated fullerenes. In principle, the above approach describes quantitatively the renormalization of the physical properties due to electron- phonon interaction and is therefore reduced by  $1+\lambda$ .

The zero temperature-limited resistivity is expressed as

$$\rho(0) = 4\pi \tau^{*-1} \omega_p^{-2}$$

From the above it is noticed that the determination of scattering rate essentially needs the Coulomb repulsive parameter, electron- phonon coupling strength, Fermi velocity, plasma frequency and upper critical magnetic field. This allows one to estimate the zero temperature-limited resistivity

independently. One uses earlier deduced values<sup>5</sup> to estimate the zero temperature elastic scattering rate which is consistent as those derived from the superconducting fluctuation measurements<sup>10</sup>. It is attributed to the fact that the larger the electron mass, the smaller the plasma frequency and hence the zero temperature elastic scattering rate.

One has earlier estimated the zero temperature mean free path,  $\ell$  about 3.4 nm which is highly sensitive for carrier scattering. One further finds that the product  $\mathcal{K}_F \ell$  ( $\sim 17$ ), seems to be much larger than unity indicates the metallic characteristics. It is worth to mention that the product,  $\varepsilon_F \tau \gg 1$ , in the test material refers to the fact that the doped fluorides fall in the weak scattering limit. This is however, consistent with the s wave superconductors. With these parameters, one estimates zero temperature limited resistivity ( $\rho_0 = 2.4 \text{ m}\Omega \text{ cm}$ ) consistent with the single crystal result<sup>10</sup>.

## NORMAL STATE RESISTIVITY

To formulate a specific model, one starts with the general expression for the temperature dependent part of the resistivity<sup>11</sup>.

$$\rho = \frac{3\pi}{\hbar e^2 v_F^2} \int_0^{2k_F} |v(q)|^2 \langle |S(q)|^2 \rangle \left( \frac{1}{2k_F} \right)^4 q^3 dq \quad (9)$$

$V(q)$  is the Fourier transform of the potential associated with one lattice site and  $S(q)$  being the structure factor. Following the Debye model it takes the following form

$$|S(q)|^2 = \frac{k_B T}{M v_s^2} f(x) \quad (10)$$

$f(x)$  being the statistical factor and to

$$f(x) = x[e^x - 1]^{-1} [1 - e^{-x}]^{-1} \quad (11)$$

Thus the resistivity expression leads to

$$\rho \approx \left[ \frac{3}{\hbar e^2 v_F^2} \right] \frac{k_B T}{M v_F^2} \int_0^{2k_F} |v(q)|^2 \left[ \frac{x q^3 dq}{(e^x - 1)(1 - e^{-x})} \right] \quad (12)$$

$V_s$  being the sound velocity. Equation (12) in terms of intermolecular phonon contribution yields the Bloch Gruneisen function of temperature dependence resistivity  $\rho$

$$\rho_{er} = (T \theta_{er}) = 4A_{er} \left( \frac{T}{\theta_{er}} \right)^4 \times T \int_0^{\theta_{er}/T} x^5 (e^x - 1)^{-1} (1 - e^{-x})^{-1} \quad (13)$$

Where  $x = \hbar \omega / k_B T$ .  $A_{er}$  being a constant of proportionality defined as

$$A_{er} \cong (3\pi^2 e^2 k_B) [\kappa_F^2 v_F^2 L \hbar v_F^2 M]^{-1} \quad (14)$$

In views of inelastic neutron scattering measurements, the phonon spectrum can be conveniently separated into two parts of phonon density of states<sup>12,13</sup>. It is natural to choose a model phonon spectrum consisting of two parts; an intermolecular phonon frequency,  $\omega_{ra}(\theta_{er})$  and an intra molecular phonon frequency,  $\omega_{ra}(\phi_{ra})$ . If the Matthiessen rule is obeyed, the resistivity may be represented as a sum  $\rho(T) = \rho_0 + \rho_{e-ph}(T)$ , where  $\rho_0$  is the residual resistivity that does not depend on temperature. On the other hand, in case of the intra molecular phonon spectrum,  $\rho_{ra}(T)$  may be described as follows

$$\rho_{ra}(T, \theta_{ra}) = A_{ra} \theta_{ra}^2 T^{-1} [\exp(\theta_{ra}/T)^{-1}]^{-1} \times [1 - \exp(-\theta_{ra}/T)]^{-1} \quad (15)$$

$A_{ra}$  is defined analogously to (14). Finally the phonon resistivity reads

$$\rho_{e-ph}(T) = \rho_{er}(T, \theta_{er}) + \rho_{ra}(T, \theta_{ra}) \quad (16)$$

Henceforth, the total resistivity is now written as

$$\begin{aligned} \rho(T, \theta_{er}, \theta_{ra}) &= \rho_0 + \rho_{er}(T, \theta_{er}) + \rho_{ra}(T, \theta_{ra}) \\ &= \rho_0 + 4A_{er}(T/\theta_{er})^4 T \times \int_0^{\theta_{er}/T} x^5 (e^x - 1)^{-1} (1 - e^{-x})^{-1} dx + \\ &A_{ra} \theta_{ra}^2 T^{-1} [\exp(\theta_{ra}/T)^{-1}]^{-1} [1 - \exp(\theta_{ra}/T)]^{-1} \end{aligned} \quad (17)$$

Though this is a purely phenomenological expression, it seems to provide a reasonable description of the available experimental data.

One also studied the temperature variation of different of resistivity

$$\rho_{diff} = [\rho_{exp} - (\rho_0 + \rho_{e-ph}\{\rho_{er} + \rho_{ra}\})] \quad (18)$$

where

- $\rho_0$  — is residual resistivity
- $\rho_{e-ph}$  — resistivity due to electron – phonon
- $\rho_{er}$  — resistivity due to intermolecular phonon
- $\rho_{ra}$  — resistivity due to intra molecular phonon

The resistivity has been studied theoretically by an approximate solution to the Boltzmann equation for the case of electron – phonon scattering mechanism<sup>14</sup>

$$\rho(T) = \frac{8\pi^2}{\omega_p^2 k_B T} \int_0^{\omega_{max}} d\omega \frac{\hbar \omega \alpha_{tr}^2 F(\omega)}{\cosh(\hbar \omega / k_B T) - 1} \quad (19)$$

where is  $\omega_p$  the plasma frequency. In the above equation the transport coupling function can be replaced by the electron – phonon coupling for superconductivity<sup>15</sup>

$$\alpha^2 F(\omega) = \frac{1}{2} \sum_v \omega_v \lambda_v \delta(\omega - \omega_v) \quad (20)$$

Due to the factor in the denominator in equation (19) phonon with frequency much larger than  $T$  do not contribute. However,

they give a linear contribution in  $T$ , if their energy is much smaller than  $k_B T$ .

### 3. DISCUSSION OF RESULTS

In this paper, using the theoretical formalism developed by Pintschovicus<sup>16</sup>, we have presented the method of evaluation of temperature variation resistivity of alkali metal doped fluoride. We have evaluated temperature variation resistivity due to electron-phonon ( $\rho_{e-ph}$ ), intermolecular phonon ( $\rho_{er}$ ) and intra molecular phonon ( $\rho_{ra}$ ), the results shown in table T<sub>2</sub>. In this evaluation we have used the value of intermolecular phonon  $\omega_{re} = 9K$  and intra molecular phonon frequency  $\omega_{ra} = 1455K$ . Our theoretical result shows that  $\rho_{er}$  increasing linearly with temperature and  $\rho_{ra}$  increasing exponentially with temperature. When both combined together then resultant resistivity  $\rho_{e-ph}$  varies exponentially at low temperature and linearly at high temperature. We have also calculated the total resistivity  $\rho(T)$  and compared our results with the experimental data. Our estimated values of  $\rho(T)$  is lower than the measured values. In this estimation we have used the model parameter  $\lambda$ ,  $\mu^*$ ,  $\nu_F$ ,  $\omega_p$ ,  $\tau$  and  $\rho_0$  which could be the reason of the lower valued of  $\rho(T)$ . We have also evaluated the temperature variation of  $\rho_{diff}$  for  $K_3C_{60}$  fluoride. From our evaluated results it appears that  $\rho_{diff}$  has power temperature dependence at low  $T$  and almost saturated values at high  $T$ . The quadratic temperature dependence at low  $T$  is an indication of conventional electron-electron scattering. This is similar to electron doped cuprates<sup>17</sup>. The departure from  $T^2$  dependence of  $\rho_{diff}$  is due to dimensionality cross over<sup>18</sup>. Thus in this paper we conclude that for the estimation of

temperature dependence resistivity in  $K_3C_{60}$ . The three scales of energy  $\omega_{er}$ ,  $\omega_{ra}$  and  $\omega_c$  (coulomb interaction) are of in same order and these are fully utilized in a model to estimate  $\rho$  which is sum of  $\rho_0$ ,  $\rho_{e-ph}$  and  $\rho_{e-e}$ . Some recent<sup>19-25</sup> studies on fluorides also reveal similar type of behavior.

**Table –T<sub>1</sub>**  
**Parameter used in the calculation**

$T_c = 22K$	$\omega_{er} = 9K$
$V_F = 1.91 \times 10^7 \text{ cm s}^{-1}$	$\omega_{re} = 1455K$
$\omega_p = 1.2 \text{ eV}$	$\rho_0 = 0.47 \text{ (m}\Omega\text{cm)}$
$HC_2(0) = 49 \text{ Tesla}$	

**Table –T<sub>2</sub>**  
**Evaluated results of temperature variation of  $\rho_{e-ph}$ ,  $\rho_{er}$  and  $\rho_{ra}$  for  $K_3C_{60}$  fluoride**

$T(K)$	$\rho_{e-ph}$ (m $\Omega$ cm)	$\rho_{er}$ (m $\Omega$ cm)	$\rho_{ra}$ (m $\Omega$ cm)
0	0.0	0.0	0.0
20	0.02	0.02	0.0
40	0.14	0.15	0.0
50	0.16	0.17	0.0
100	0.22	0.25	0.0
200	0.78	0.50	0.22
300	2.5	0.70	1.52

**Table –T<sub>3</sub>**  
**An evaluated results of temperature variation of total resistivity  $\rho(T)$  of  $K_3C_{60}$**

$T(K)$	$\rho(T)$ (m $\Omega$ cm)	
	Theory	Expt.
0	0.0	0.0
25	2.50	2.62
50	2.55	2.76
100	2.75	3.16
200	3.00	3.90
300	4.00	4.51

**Table –T<sub>4</sub>****An evaluated results of temperature variation**

of  $\rho_{diff} = [\rho_{exp} - \{\rho_o + \rho_{e-ph} (= \rho_{er} + \rho_{ra})\}]$   
**for alkali metal doped fluoride K<sub>3</sub>C<sub>60</sub>.**

Temperature T <sup>2</sup> (10 <sup>4</sup> K <sup>2</sup> )	$\rho_{diff} = [\rho_{exp} - \{\rho_o + \rho_{e-ph} (= \rho_{er} + \rho_{ra})\}]$	
	Theoretical (mΩcm)	Linear Fit (mΩcm)
0	0.125	0.132
1.0	0.110	0.156
2.0	0.268	0.295
3.0	0.455	0.462
4.0	0.622	0.656
5.0	0.668	0.575
6.0	0.585	0.853

**REFERENCES**

1. B.Burk, V. H. Crespi, A. Zettl and M. L. Cohen, *Phys. Rev. Lett. (PRL)* 72, 3706 (1994).
2. E.Cappelluti, C. Grimaldi, L. Pietronero and S. Strassler, *Phys. Rev. Lett.(PRL)* 85, 4771 (2000).
3. E. Cappelluti, C. Grimaldi, L. Pietronero, S. Strassler and G. A. Ummrino, *Eur. Phys. JB21*, 383 (2001).
4. V. H. Crespi and M. L. Cohen, *Phys. Rev. B53*, 56 (1996).
5. G. Sparn, J. D. Thompson, R. L. Whetten, S. M. Huang, R. B. Kaner and K. Holczer, *Science* 252, 1829 (1991).
6. G. Sparn, J. D. Thompson, R. L. Whetten, S. M. Huang, R. B. Kaner and K. Holczer, F.Diederich and G. Gruner, *Phys. Rev. Lett. (PRL)* 68, 1228 (1992).
7. S. Satapathy, V. O. Antropov, O. K. Anderson, O. Jepsen and I. Liechten-sion, *Phys. Rev. B46*, 1773 (1992).
8. J. P. Carbotte, *Rev. Mod. Phys.* 62, 11012 (1990).
9. V. H. Crespi, J. G. Hou, X. D. Xiang, M. L. Cohen and A. Zettl, *Phys. Rev. B46*, 12064 (1992).
10. X. D. Xiang, J. G. Hou, G. Briceno, W. A. Walecka, R. Mostovoy, V. H. Crespi and M. L. Cohen, *Science* 256, 1190 (1992).
11. G. Grimvall, 'Electron- Phonon Interaction in Metals (North-Holland Publishing Company, Netherlands (1981).
12. D. L. Novikov, V. A. Gubanov and A. J. Freeman, *Physica C191*, 399 (1992).
13. T. T. M. Palstra, R. C. Haddon, A. F. Hebard and J. Zaaren, *Phys. Rev. Lett. (PRL)* 64, 1054 (1992).
14. D. Varshney, J. Superconductivity 13, 171 (2000).
15. D. Varshney, K. K. Choudhary and R. K. Singh, *Supercond. Sci. Technol* 15, 1119 (2002).
16. L. Pintschovius, *Rep. Prog. Phys.* 59, 473 (1996).
17. D. Varshney and R. K. Singh, *Physica C282-287*, 1919 (1997).
18. T. S. Chida, S. Suzuki and K. Nakao, *J. Phys. Soc. Jpn.* 71, 525 (2002).
19. V. H. Crespi and M. L. Cohen, *Phys. Rev. B53*, 46 (1996).
20. K. Nakao, M. P. Gelfed, S. Suzuki, T. T. M. Palstra and T. S. Chida, *J. Phys. Soc. Jpn.* 76, 123 (2004).
21. R. J. C. Batista, M. S. C. Mazzoni and H. Chachem, *Chemical Physics Letters.* 421, 246 (2006).
22. L. M. Wang, R. Pal, W. Huang, C. Zeng and L. S. Wang, *The Journal of Chemical Physics* 130, 051101 (2009).
23. L. M. Ramanich and M. Boero, *The Journal of Chemical Physics*, 133, 134701 (2010).
24. E. Neyts, A. Maeyens, G. Pourtois and A. Bogaerts, *Carbon* 49, 1013 (2011).
25. F. Naderi, S. Rostamian and B. Naderi, *International Journal of Physical Sciences* 7(13), 2006 (2012).